Specification

Title of the Invention

Simulation Calculation Service Providing Method, System, and Storage Medium Which Stores Program

5

Background of the Invention

The present invention relates to a simulation calculation service providing system which efficiently operates the simulation technology in each field by IT

10   (Information Technology).

The conventional simulation technology has been used by causing some experts to independently prepare simulation calculation programs and computers, access computer centers via, e.g., telnet, or visit the

15   computer centers to activate, on computers, simulation calculation programs resident at the centers.

The conventional technology however has the following problems.

To use the simulation technology by

20   independently preparing simulation calculation programs and computers, users must prepare the hardware and software by themselves. Since the initial investment is enormous, the users are limited to well-funded simulation experts and research workers familiar to the

25   simulation technology.

Additionally, since the users hold themselves responsible for the change/upgrading of application

- 1 -

software, the maintenance, and the handling of accidents, they are required to have competences to some extent or more.

To use the simulation technology by accessing a computer center via telnet or the like, each user must prepare a server to be used to connect the Internet. This requires initial investment.

To use the simulation technology by activating, on a computer, a simulation calculation program that is resident at a computer center, the user must directly visit the computer center, and it is time-consuming.

As described above, there are high hurdles to be got over to use the simulation technology. For many other research workers who are potential users of the simulation technology, for example, temporary users and non-experts, it is substantially impossible to actually use the simulation technology.

Summary of the Invention

It is an object of the present invention to provide a simulation calculation service providing method and system which can increase opportunities to use simulation calculation and can easily be used on the basis of user's requests, and a storage medium which stores a program therefor.

In order to achieve the above object, according to the present invention, there is provided a

- 2 -

simulation calculation service providing method of providing simulation calculation in a server system connected to a user terminal apparatus and a consultant terminal apparatus through a network, comprising the

5 steps of receiving a condition of the simulation calculation from the user terminal apparatus as a user presented condition, registering the received user presented condition, receiving, from the consultant terminal apparatus, a bidding condition from a

10 consultant in correspondence with the registered user presented condition, comparing the user presented condition with the bidding condition and selecting a bidding condition that coincides with the user presented condition, inquiring of the user terminal apparatus

15 about whether the simulation calculation is to be executed on the basis of the selected bidding condition, and executing the simulation calculation in accordance with an answer to the inquiry.

Brief Description of the Drawings

20 Fig. 1 is a block diagram showing the arrangement of a simulation calculation service providing system according to an embodiment of the present invention;

Fig. 2 is a block diagram for explaining the

25 arrangement of a server system according to the embodiment of the present invention;

Fig. 3 is a flow chart showing an operation of.

executing simulation calculation by using a simulation calculation service providing system according to the first embodiment of the present invention;

Fig. 4 is a flow chart showing an operation of executing simulation trial calculation by using a simulation calculation service providing system according to the second embodiment of the present invention;

Fig. 5 is a flow chart showing an operation of executing simulation calculation related to proteins by using the simulation calculation service providing system according to the first embodiment of the present invention;

Fig. 6 is a flow chart showing the operation of executing simulation calculation related to proteins by using the simulation calculation service providing system according to the first embodiment of the present invention;

Fig. 7 is a flow chart showing the operation of executing simulation calculation related to proteins by using the simulation calculation service providing system according to the first embodiment of the present invention;

Fig. 8 is a flow chart showing the operation of executing simulation calculation related to proteins by using the simulation calculation service providing system according to the first embodiment of the present

invention;

Fig. 9 is a flow chart showing an operation of executing simulation trial calculation related to proteins by using the simulation calculation service providing system according to the second embodiment of the present invention;

Fig. 10 is a flow chart showing the operation of executing simulation trial calculation related to proteins by using the simulation calculation service providing system according to the second embodiment of the present invention;

Fig. 11 is a flow chart showing the operation of executing simulation trial calculation related to proteins by using the simulation calculation service providing system according to the second embodiment of the present invention; and

Fig. 12 is a flow chart showing the operation of executing simulation trial calculation related to proteins by using the simulation calculation service providing system according to the second embodiment of the present invention.

Description of the Preferred Embodiments

The embodiments of the present invention will be described next in detail with reference to the accompanying drawings.

The same reference numerals denote parts having the same functions throughout the drawings for

explaining the embodiments, and a repetitive description will be omitted.

As shown in Fig. 1, a simulation calculation service providing system according to an embodiment of the present invention comprises a user terminal apparatus 5, consultant terminal apparatus 7, and server system 1. The server system 1 is constituted by a user management apparatus 2, simulation analysis apparatus 3, and consultant management apparatus 4.

The user terminal apparatus 5 comprises a control section 5e, and a communication section 5a, operation section 5b, storage section 5c, and display section 5d which are connected to the control section 5e.

The communication section 5a communicates information to the server system 1 through a network 6 such as the Internet. The operation section 5b inputs a received user's request or instruction to the control section 5e. The operation section 5b comprises at least one of, e.g., a browser, a graphical user interface, and any other input means and inputs a request or instruction by using the input means. The storage section 5c stores a program for the control section 5e, a browser, and a program which causes the user terminal apparatus 5 to execute functions installed in it. The storage section 5c inputs/outputs data to/from the control section 5e. The display section 5d is

constituted by a display device such as an LCD. The
display section 5d is controlled by the control section
5e to display a simulation condition input window or a
simulation calculation result received from the server
5   system 1. The control section 5e systematically
controls the respective sections of the user terminal
apparatus 5 on the basis of, e.g., a program.

The user terminal apparatus 5 is constituted
by, e.g., a personal computer (PC), a cellular phone, or
10   a PDA (Personal Digital Assistance). When the user
terminal apparatus 5 is constituted by, e.g., a personal
computer, a browser stored in the storage section of the
personal computer is activated. Then, the address of
the user management apparatus 2 (to be described later)
15   is input to access it.

The consultant terminal apparatus 7 is a
terminal apparatus similar to the user terminal
apparatus 5. The consultant terminal apparatus 7
comprises a control section 7e, and a communication
20   section 7a, operation section 7b, storage section 7c,
and display section 7d which are connected to the
control section 7e.

The communication section 7a communicates
information to the server system 1 through the network 6
25   such as the Internet. The operation section 7b inputs a
received consultant's request or instruction to the
control section 7e. The operation section 7b comprises

at least one of, e.g., a browser, a graphical user interface, and any other input means and inputs a request or instruction by using the input means. The storage section 7c stores a program for the control section 7e, a browser, and a program which causes the consultant terminal apparatus 7 to execute functions installed in it. The storage section 7c inputs/outputs data to/from the control section 7e. The display section 7d is constituted by a display device such as an LCD. The display section 7d is controlled by the control section 7e to display a bidding condition input window or a simulation calculation result received from the server system 1. The control section 7e systematically controls the respective sections of the consultant terminal apparatus 7 on the basis of, e.g., a program.

The consultant terminal apparatus 7 is constituted by, e.g., a personal computer (PC), a cellular phone, or a PDA (Personal Digital Assistance), like the user terminal apparatus 5. When the consultant terminal apparatus 7 is constituted by, e.g., a personal computer, a browser stored in the storage section of the personal computer is activated. Then, the address of the consultant management apparatus 4 (to be described later) is input to access it.

The server system 1 will be described next. The server system 1 is constituted by the user

management apparatus 2, simulation analysis apparatus 3, and consultant management apparatus 4.

The user management apparatus 2 will be described first.

The user management apparatus 2 comprises a communication IF section 2-1, transmission/reception section 2-2, authentication/registration section 2-3, user DB (database) 2-4, information management section 2-5, storage section 2-6, calculation control section 2-7, estimation section 2-8, charging section 2-9, and encryption section 2-2a.

The communication IF section 2-1 is an interface to be used to transmit/receive data to/from the user terminal apparatus 5 through the network 6 such as the Internet. The communication IF section 2-1 is connected in parallel with a plurality of user terminal apparatuses 5 on the network 6.

The transmission/reception section 2-2 inputs/outputs data to/from the authentication/registration section 2-3, the calculation control section 2-7, and a trial calculation section 2-10 (to be described later) in accordance with a connection request from the user terminal apparatus 5. For example, the transmission/reception section 2-2 is connected to the authentication/registration section 2-3 in accordance with a connection request from the user terminal apparatus 5. In addition, the

transmission/reception section 2-2 receives, as user

presented conditions, simulation calculation conditions

and request items related to the simulation calculation

and inputs them to the calculation control section 2-7

5   or trial calculation section 2-10 (to be described

later). The transmission/reception section 2-2 also

inputs, to the information management section 2-5, an

automatic price estimation result output from the

estimation section 2-8. The transmission/reception

10   section 2-2 also inputs, to the information management

section 2-5, a simulation calculation result output from

the calculation control section 2-7. The

transmission/reception section 2-2 also inputs, to the

information management section 2-5, a simulation trial

15   calculation result output from the trial calculation

section 2-10.

        The authentication/registration section 2-3

comprises an authentication section 2-3a and

registration section 2-3b.

20   The authentication section 2-3a causes a user

who has already been registered as a member to input at

least a system registration ID (identification) and a

password to execute member authentication, and transmits

a message representing use permission to the user who is

25   granted permission to use by member authentication.

Also, in accordance with a request from the user who is

granted permission to use, the authentication section

2-3a transmits application software information and the input information of data necessary for the use of the application software to the user terminal apparatus 5.

The registration section 2-3b registers a user who wants to be registered as a member or a non-member user who wants to use the system by way of trial.

The user DB (database) 2-4 is a database which stores the information of users who have already been registered as members. When a user inputs his/her system registration ID and password in an authentication/registration window, the authentication section 2-3a executes authentication processing to determine whether the user who has input the system registration ID and password can use the system.

The information management section 2-5 registers, in the storage section 2-6 (to be described later), a price estimation result output from the estimation section 2-8 and a simulation calculation result output from the calculation control section 2-7. In response to an access request from the user terminal apparatus 5, the information management section 2-5 transmits an acknowledge signal for requested information.

The storage section 2-6 stores user presented conditions and simulation calculation result input from the information management section 2-5.

The calculation control section 2-7 executes

control in simulation calculation. The calculation control section 2-7 inputs user presented conditions designated by the user to the estimation section 2-8 (to be described later). The calculation control section 2-7 also receives a simulation result output from the simulation analysis apparatus 3 (to be described later).

The estimation section 2-8 comprises a price estimation section 2-8a. The price estimation section 2-8a estimates the price of simulation calculation on the basis of user presented conditions output from the calculation control section 2-7. As will be described later, the estimation section 2-8 also comprises a calculation capability determination section 2-8b which determines whether simulation calculation goes beyond the upper limit of the processing capability (computation capability) of the system when a user is going to use the simulation calculation service providing system by way of trial.

The charging section 2-9 charges a fee for the use of the system. For example, the charging section 2-9 charges a user who uses the system.

The trial calculation section 2-10 executes control for simulation trial calculation. The trial calculation section 2-10 inputs user presented conditions designated by the user to the estimation section 2-8. The trial calculation section 2-10 also inputs a simulation result output from the simulation

analysis apparatus 3 to the transmission/reception section 2-2.

The encryption section 2-2a is arranged in the transmission/reception section 2-2 to encrypt information to be transmitted/received, i.e., inquiries, user presented conditions, bidding conditions, replies to inquiries, and the like.

The simulation analysis apparatus will be described next.

The simulation analysis apparatus 3 comprises a matching section 3-1, simulation section 3-2, and simulation result analysis section 3-3.

The matching section 3-1 is constituted by a comparison section 3-1a, selection section 3-1b, and inquiry section 3-1c. The comparison section 3-1a compares user presented conditions received from the estimation section 2-8 with bidding conditions designated by a consultant who has referred to the user presented conditions. The selection section 3-1b selects bidding conditions that are determined by the comparison section 3-1a to coincide with (match) the user presented conditions. The inquiry section 3-1c inquires of the user terminal apparatus 5 about whether simulation calculation should be executed on the basis of the bidding conditions selected by the selection section 3-1b. If the answer to this inquiry is "OK", the inquiry section 3-1c inputs the matching simulation

calculation conditions to the simulation section 3-2.

The simulation section 3-2 is constituted by a computer group having one or a plurality of computers and an application software group having one or a

5 plurality of pieces of application software.

The simulation section executes simulation calculation on the basis of the conditions input from the matching section 3-1 by using the hardware of the computer group and the application software of the

10 application software group. The simulation section inputs the simulation calculation result to the simulation result analysis section 3-3.

The computer group may be prepared by a public organization such as a state or a community comprised of

15 one or a plurality of companies that are planning business using simulation. The operation cost may be covered with fees for the computers, which are paid by consultants or users. The application software group may be provided by simulation experts or IT operators.

20 Alternatively, it may be provided to penetrate developed simulation technologies or software and prove their effectiveness. In this case, a corresponding value may be paid by the operator who is operating the system.

The simulation result analysis section 3-3

25 temporarily stores the simulation calculation result output from the simulation section 3-2 and transmits a copy of the simulation calculation result to the

consultant management apparatus 4 (to be described later).

The simulation result analysis section 3-3 also receives intellectual added value information such as an analysis result added by the consultant who has referred to the simulation calculation result and transmits the intellectual added value information to the user terminal apparatus 5 together with the simulation calculation result.

The consultant management apparatus 4 will be described next.

The consultant management apparatus 4 comprises a communication IF section 4-1, transmission/reception section 4-2, authentication/registration section 4-3, consultant DB 4-4, information management section 4-5, storage section 4-6, and money reception section 4-7.

The communication IF section 4-1 is an interface to be used to transmit/receive data to/from the consultant terminal apparatus 7 through the network 6 such as the Internet. The communication IF section 4-1 is connected in parallel with a plurality of consultant terminal apparatuses 7 on the network 6.

The transmission/reception section 4-2 inputs/outputs data to/from the authentication/registration section 4-3 (to be described later), matching section 3-1, and simulation result

analysis section 3-3 in accordance with a request from the consultant terminal apparatus 7. For example, the transmission/reception section 4-2 is connected to the authentication/registration section 4-3 in accordance

5   with a connection request from the consultant terminal apparatus 7. In addition, the transmission/reception section 4-2 receives user presented conditions from the matching section 3-1 and inputs them to the information management section 4-5 (to be described later). The

10   transmission/reception section 4-2 also receives a simulation calculation result for the simulation result analysis section 3-3 and transmits it to the consultant terminal apparatus 7. The transmission/reception section 4-2 also receives intellectual added value

15   information from the consultant terminal apparatus 7 and transmits it to the simulation result analysis section 3-3.

          The transmission/reception section 4-2 also registers new application software or changes/upgrades

20   application software in the simulation section 3-2.

          The authentication/registration section 4-3 comprises an authentication section 4-3a and registration section 4-3b.

          The authentication section 4-3a causes a

25   consultant who has already been registered as a member to input at least a system registration ID (identification) and a password to execute member

- 16 -

authentication, and transmits a message representing use permission to the consultant who is granted permission to use by member authentication.

The registration section 4-3b registers a non-member consultant who will use the system.

The consultant DB (database) 4-4 is a database which stores the information of consultants who have already been registered as members. When a consultant inputs his/her system registration ID and password in an authentication/registration window, the authentication/registration section 4-3 executes authentication processing to determine whether the consultant who has input the system registration ID and password can use the system.

The information management section 4-5 stores, in the storage section 4-6 (to be described later), user presented conditions output for the matching section 3-1 and a simulation calculation result output from the simulation result analysis section 3-3. In response to an access request from the consultant terminal apparatus 7, the information management section 4-5 transmits an acknowledge signal for requested information.

The storage section 4-6 stores user presented conditions and simulation calculation result input from the information management section 4-5.

The money reception section 4-7 receives compensation for a consultant. For example, an amount

obtained by deducting a commission from an amount paid by a user is paid as compensation by the operation entity that operates the system.

The arrangement of the server system 1 according to this embodiment will be described next.

As shown in Fig. 2, the server system 1 is constituted by an input/output device 8, display device 9, drive device 10, storage medium 11, auxiliary storage device 12, memory device 13, arithmetic processing device 14, database (DB) 15, and IF device 16. The interface (IF) device 16 is connected to the user terminal apparatus 5 and consultant terminal apparatus 7 through the network 6.

The input/output device 8 is formed from a keyboard and mouse operated by the manager of the server system 1, and used to input various operation signals to the server system 1.

The display device 9 displays various kinds of windows and data necessary for operating the server system 1.

The interface device 16 is an interface used to connect the server system 1 to the network 6 and is formed from, e.g., a modem.

The database 15 is designed to include, e.g., the user DB 2-4 and consultant DB 4-4.

A simulation calculation service providing program related to the simulation calculation service

providing system is provided by a software package,
i.e., the information storage medium 11 such as a
CD-ROM, ROM, RAM, flexible disk, or memory card. When
the storage medium 11 which stores the simulation

5   calculation service providing program is set in the
drive device 10, the program is installed from the
storage medium 11 to the auxiliary storage device 12
through the drive device 10.

The auxiliary storage device 12 stores the

10   installed simulation calculation service providing
program and also necessary files and data.

At the time of activating the server system,
the memory device 13 reads out the simulation
calculation service providing program from the auxiliary

15   storage device 12 and stores the program.

The simulation calculation service providing
program may be provided through telecommunication, and
for example, by a server.

The arithmetic processing device 14 executes

20   processing of the simulation calculation service
providing system in accordance with the simulation
calculation service providing program read out and
stored in the memory device 13.

The processing of the simulation calculation

25   service providing system according to this embodiment
will be described next with reference to Fig. 3.

The user operates the user terminal apparatus

5 and activates a browser stored in the storage section
5c to access the user management apparatus 2 through the
network 6.

The authentication/registration section 2-3 of
5   the user management apparatus 2 confirms whether the
user who is accessing it has already been registered
(S301).

If user registration is not executed yet (NO
in S301), a notification representing that the user
10   should be registered is sent (S302), and user
registration is performed (S303).

When the user has already been registered (YES
in S301), a user authentication window is displayed.
The user inputs the user ID and password, and after
15   authentication processing is done, logs in (S304).

When the user is granted permission to use as
a result of authentication processing, a window in which
simulation conditions and request items related to
simulation calculation are to be input is displayed on
20   the display section 5d of the user terminal apparatus 5
that is accessing the user management apparatus 2. The
user inputs desired simulation calculation conditions
and request items.

For example, an edit box in which simulation
25   calculation conditions and request items related to
simulation calculation are to be input and a command
button "transmit" are displayed. The user inputs

- 20 -

simulation calculation conditions and request items to the blank field of the edit box. When input is ended, the user clicks on the "transmit" button by using, e.g., the mouse. Accordingly, the simulation calculation

5   conditions and request items are transmitted to the user management apparatus 2.

The transmitted simulation conditions and request items are received by the transmission/reception section 2-2 as user presented conditions (S305). The

10   user presented conditions received by the transmission/reception section 2-2 are input to the calculation control section 2-7. The user presented conditions are input from the calculation control section 2-7 to the estimation section 2-8. The

15   estimation section 2-8 automatically estimates the price of simulation on the basis of the received user presented conditions (S306). The estimation result is input to the transmission/reception section 2-2. The transmission/reception section inputs the received price

20   estimation result to the information management section 2-5. The information management section 2-5 registers the received price estimation result in the storage section 2-6 and presents the price (S307). The user terminal apparatus 5 can refer to the price estimation

25   result by accessing the information management section 2-5.

The user refers to the price estimation result

and examines whether the simulation calculation is to be continued or the system is to be ended without executing the simulation calculation. When the simulation calculation should be continued, the user examines

5   whether the simulation calculation should be executed on the basis of the current conditions or re-examines the simulation calculation conditions, and transmits the examination result. This operation is done by, e.g., displaying the simulation condition input window again

10   and causing the user to input simulation conditions again.

The examination result transmitted from the user terminal apparatus 5 is received by the transmission/reception section 2-2 of the user

15   management apparatus 2 (S308).

When the examination result indicates that the simulation calculation should be continued (YES in S309), the simulation calculation conditions are input from the transmission/reception section 2-2 to the

20   estimation section 2-8 through the calculation control section 2-7.

When the received examination result indicates that no simulation calculation should be executed (NO in S309), the system is ended (S309).

25   The estimation section 2-8 estimates the price again on the basis of the newly input user presented conditions. The estimation result is transmitted to the

matching section 3-1 of the simulation analysis
apparatus 3 together with the user presented conditions
(S310).

The user presented conditions and price
estimation result transmitted to the matching section
3-1 are transmitted to the transmission/reception
section 4-2 of the consultant management apparatus 4.
Upon receiving the user presented conditions and price
estimation result, the transmission/reception section
4-2 inputs the user presented conditions and price
estimation result to the information management section
4-5. The information management section 4-5 registers
the received user presented conditions and automatic
price estimation result in the storage section 4-6.

On the other hand, a single consultant or each
of a plurality of consultants operates the consultant
terminal apparatus 7 connected to the consultant
management apparatus 4 through the network 6 and
activates a browser stored in the storage section to
access the consultant management apparatus 4. The
authentication/registration section 4-3 confirms whether
the consultant who is accessing it has already been
registered as a consultant.

If consultant registration is not executed
yet, the registration section sends a notification
representing that the consultant should be registered
and performs consultant registration.

A notification representing the presence/absence of matters presented by users may be automatically transmitted to registered consultants by email or the like. Alternatively, the matters may be

5   open to the public on homepages or the like.

When the consultant has already been registered, a user authentication window is displayed. The consultant inputs the consultant ID and password and logs in.

10   When the consultant is granted permission to use as a result of authentication processing, the transmission/reception section 4-2 accesses the information management section 4-5. Consequently, a list of user presented conditions and automatic price

15   estimation results is displayed on the display screen of the consultant terminal apparatus 7. The consultant selects user presented conditions and an automatic price estimation result, for which he/she wants to offer consultations, from the list of user presented

20   conditions and automatic price estimation results, and inputs and transmits bidding conditions on the basis of the selected user presented conditions and automatic price estimation result.

The bidding conditions transmitted from the

25   consultant terminal apparatus 7 are received by the transmission/reception section 4-2 of the consultant management apparatus 4 (S311) and transmitted to the

matching section 3-1 of the simulation analysis apparatus 3.

The matching section 3-1 compares the user presented conditions with bidding conditions, selects bidding conditions that coincide with (match) the user presented conditions, and inquires of the user terminal apparatus 5 about whether simulation calculation is to be executed on the basis of the selected bidding conditions.

If the answer to this inquiry is "OK" (YES in S312), simulation calculation conditions of the user presented conditions that coincide with the bidding conditions are input to the simulation section (S313).

The simulation section 3-2 automatically executes simulation calculation on the basis of the received simulation calculation conditions (S314).

The simulation calculation result is input to the simulation result analysis section 3-3 and temporarily stored (S315). A copy of the simulation calculation result is sent to the consultant who has got the contract (made a successful bid) for the simulation calculation through the consultant terminal apparatus 7 (S316).

The consultant adds intellectual added value information such as an analysis result or the explanation of the result while referring to the received simulation calculation result and returns the

intellectual added value information to the simulation
result analysis section 3-3.

Upon receiving the intellectual added value
information (S317), the simulation result analysis
section 3-3 temporarily stores it (S318) and transmits
the received intellectual added value information and
the simulation calculation result to the user terminal
apparatus 5 (S319).

A case wherein the user is to use the
simulation calculation service providing system by way
of trial will be described next with reference to
Fig. 4.

The user operates the user terminal apparatus
5 and activates a browser stored in the storage section
5c to access the user management apparatus 2 through the
network 6.

The authentication/registration section 2-3 of
the user management apparatus 2 executes user
registration for the user who is accessing it (S401).

User authentication may be performed after
user registration (S402).

When the user is granted permission to use as
a result of authentication processing, a window in which
simulation conditions and request items related to
simulation calculation are to be input is displayed on
the display section of the user terminal apparatus 5
that is accessing the user management apparatus 2. The

user inputs desired simulation calculation conditions
and request items.

For example, an edit box in which simulation
calculation conditions and request items related to
5   simulation calculation are to be input and a command
button "transmit" are displayed. The user inputs
simulation calculation conditions and request items to
the blank field of the edit box. When input is ended,
the user clicks on the "transmit" button by using, e.g.,
10 the mouse. Accordingly, the simulation calculation
conditions and request items are transmitted to the user
management apparatus.

The transmitted simulation conditions and
request items are received by the transmission/reception
15 section 2-2 as user presented conditions (S403). The
user presented conditions received by the
transmission/reception section 2-2 are input to the
trial calculation section 2-10. The user presented
conditions are input from the trial calculation section
20 2-10 to the estimation section 2-8. The estimation
section 2-8 estimates the price of simulation
calculation on the basis of the received user presented
conditions and determines whether the simulation
calculation goes beyond the upper limit of the
25 processing capability (computation capability) of the
system (S404). The result is input to the
transmission/reception section 2-2. The

transmission/reception section 2-2 inputs the received

estimation result to the information management section

2-5. The information management section 2-5 stores the

received estimation result in the storage section 2-6

5   (S405). The user can refer to the estimation result by

operating the user terminal apparatus 5 and accessing

the information management section 2-5.

The user refers to the estimation result and

examines whether the simulation trial calculation is to

10   be continued or the system is to be ended without

executing the simulation trial calculation. When the

simulation trial calculation should be continued, the

user examines whether the simulation trial calculation

should be executed on the basis of the current

15   conditions or re-examines the simulation trial

calculation conditions, and transmits the examination

result. This operation is done by, e.g., displaying the

simulation condition input window again and causing the

user to input simulation conditions again.

20   The examination result transmitted from the

user terminal apparatus 5 is received by the

transmission/reception section 2-2 of the user

management apparatus 2 (S406).

When the examination result indicates that the

25   simulation trial calculation should be continued (YES in

S407), the simulation trial calculation conditions are

input from the transmission/reception section 2-2 to the

estimation section 2-8 through the trial calculation section 2-10.

When the received examination result indicates that no simulation trial calculation should be executed (NO in S407), the system is ended.

On the basis of the newly input user presented conditions, the estimation section 2-8 automatically estimates the price and determines whether the simulation trial calculation goes beyond the upper limit of the processing capability of the system (S408). If the simulation trial calculation goes beyond the upper limit of the processing capability of the system, and trial calculation cannot be executed, the system is ended (NO in S408).

When the simulation trial calculation falls within the limit of the processing capability of the system, and trial calculation can be executed (YES in S408), the simulation calculation conditions are input to the simulation section 3-2 (S409).

The simulation section 3-2 automatically executes the simulation calculation on the basis of the received simulation calculation conditions (S410).

The simulation calculation result is input to the simulation result analysis section 3-3 and temporarily stored (S411). A copy of the simulation calculation result is sent to the consultant who has got the contract for the simulation calculation through the

consultant terminal apparatus 7 (S412).

The consultant adds intellectual added value information such as an analysis result or the explanation of the result while referring to the

5   received simulation calculation result and returns the intellectual added value information to the simulation result analysis section 3-3.

Upon receiving the intellectual added value information (S413), the simulation result analysis

10   section 3-3 temporarily stores it (S414) and transmits the received intellectual added value information and the simulation calculation result to the user terminal apparatus 5 (S415).

An example will be described next with

15   reference to Figs. 5 to 8, in which when target protein function control which is effective in the drug design field is to be executed by using the above-described simulation calculation service providing system, pieces of information about portions of the target protein, to

20   which molecules as drug candidates bind, and the difference in affinity to the respective portions are to be collected.

The user operates the user terminal apparatus 5, activates a browser stored in the storage section 5c,

25   and, for example, designates the address of the user management apparatus 2 on the browser to access the user management apparatus 2 through the network 6 such as the

Internet.

The authentication/registration section 2-3 of the user management apparatus 2 confirms whether the user who is accessing it has already been registered (S501).

If user registration is not executed yet (NO in S501), a notification representing that the user should be registered is sent, and user registration is performed (S502). The user registration may be charged.

When the user has already been registered (YES in S501), a user authentication window is displayed. The user inputs the user ID and password and logs in (S503).

When the user is granted permission to use as a result of authentication processing, a window in which simulation calculation conditions and request items related to simulation calculation are to be input is displayed on the display section 5d of the user terminal apparatus 5 that is accessing the user management apparatus 2. The user inputs desired simulation calculation conditions and request items related to the simulation calculation.

Table 1 User Presented Conditions

Delivery Time	Price	Contents of Simulation Calculation				Priority Item
		Three-Dimensional Structure	Energy	Property	Docking	
30	200	YES	YES	YES	YES	Delivery time
		YES	YES	YES		
Number of amino acid residues	Number of atoms	Composition	Three-dimensional structure information	Sequence information	Homology	Binding site
100	1500	Amino acid	UNKNOWN	UNKNOWN	UNKNOWN ·	UNKNOWN

- 31 -

-	60	Organic	UNKNOWN	-	-	10

For example, simulation calculation conditions
and request items related to simulation calculation in
molecular binding simulation (docking simulation)

5   include "contents of simulation calculation",
"information about molecules to be calculated",
"delivery time", "price", "priority item", and "rank",
as shown in Table 1. The request items can be added or
changed by the manager or user of the system, as needed.

10   The contents of simulation calculation include
"three-dimensional structure predictive calculation
(three-dimensional structure)", "three-dimensional
structure predictive calculation and energy calculation
(energy)", "physical quantity (property) calculation"

15   such as electrostatic potential calculation, and
"molecular binding simulation (docking simulation)".
When molecular binding simulation is to be executed, the
number of binding site candidate portions of a protein
molecule, where docking simulation should be executed,

20   is designated.

Information about molecules to be calculated
contains "number of amino acid residues", "number of
atoms", "composition", "three-dimensional structure
information", "sequence information", "homology", and

25   "binding site".

For example, "composition" designates whether
a molecule is comprised of an amino acid.

"Three-dimensional structure information" designates
whether the three-dimensional structure is known.
"Sequence information" designates whether the sequence
information is known. "Homology" designates whether the
5 presence/absence of homology is known. "Binding site"
designates whether the binding site is known or the
number of binding site candidate portions where
calculation should be executed. These pieces of
information are designated for each of the target
10 molecule and substrate molecule.

"Priority item" is an item which has high
priority in comparing user presented conditions with
bidding conditions designated by a consultant who has
referred to the user presented conditions and selecting
15 bidding conditions that coincide with (match) the user
presented conditions. "Priority item" includes items
designated in the user presented conditions, and here,
"delivery time", "price", and "contents of simulation
calculation".

20 "Rank" is an index to be used to identify the
technical capability of each consultant. Each
consultant is given a rank at the time of registration.
For example, A, B, and C are given as ranks in
descending order of technical capability of consultants.
25 The rank changes in accordance with the actual
performance in this system.

In this embodiment, "delivery time" is

designated on a day-by-day basis. "Price" is designated in steps of 1 dollar. "Three-dimensional structure", "property", "energy", and "docking" are designated by YES/NO. "Three-dimensional structure information",

5 "sequence information", "homology", and "binding site" are designated by KNOWN/UNKNOWN.

For "binding site", the number of binding sites for which docking simulation is to be executed. When "binding site" is UNKNOWN, the number of sites to

10 be calculated is designated. When "binding site" is KNOWN, the number of known sites is designated.

In the user presented conditions shown in Table 1, "delivery time" is 30 days, and "price" is 200 dollar. In "contents of simulation calculation", both

15 the target molecule and substrate molecule are designated as "YES" in "three-dimensional structure predictive calculation", "energy calculation (energy)", "physical quantity (property)", and "molecular binding simulation (docking simulation)". "Priority item" is

20 "delivery time".

In "information about molecules to be calculated", for the target molecule, "number of amino acid residues" is 100, "number of atoms" is 1,500, "composition" is amino acid, "three-dimensional

25 structure information" is UNKNOWN, "sequence information" is UNKNOWN, "homology" is UNKNOWN, and "binding site" is UNKNOWN. For the substrate molecule,

- 34 -

"number of atoms" is 60, "composition" is organic,
"three-dimensional structure information" is UNKNOWN,
and "number of sites to be calculated" is 10.

The transmitted simulation calculation
5   conditions and request items are received by the
transmission/reception section 2-2 as user presented
conditions (S504). The user presented conditions
received by the transmission/reception section 2-2 are
input to the calculation control section 2-7. The user
10   presented conditions are input from the calculation
control section 2-7 to the estimation section 2-8.

The estimation section 2-8 automatically
estimates the price of simulation calculation on the
basis of the received user presented conditions (S505).
15   The estimation section 2-8 roughly estimates the
calculation time on the basis of the received user
presented conditions by using a molecular simulation
method such as homology search or a method of molecular
orbitals/molecular dynamics. The estimation section 2-8
20   also automatically roughly estimates the price
corresponding to the calculation contents. For example,
the price is automatically calculated from an estimated
CPU processing time, and for example, an estimated
calculation time and a point defined in advance in
25   correspondence with the level of calculation contents.

A plurality of price estimation results are
presented on the basis of the priority item designated

in the user presented conditions. In the plurality of estimated conditions presented to the user, items except the priority item designated in the user presented conditions do not always match the user's desired

5   conditions.

Table 2   Price Estimation Results

Delivery Time	Price	Contents of Simulation Calculation				Binding Site
		Three-Dimensional Structure	Energy	Property	Docking	
14	150	YES	YES	YES	NO	0
		YES	YES	YES		
21	300	YES	YES	YES	YES	10
		YES	YES	YES		
30	400	YES	YES	YES	YES	10
		YES	YES	YES		
Immediate	1000	YES	NO	YES	NO	0
		YES	NO	YES		

As shown in Table 2, the price estimation result includes, e.g., "delivery time", "price", "contents of simulation calculation", and "binding

15   site".

For the delivery time, since the priority item designated in the user presented conditions in Table 1 is "delivery time" of 30 days, price estimations that satisfy the delivery time of 30 days are displayed.

20   For "price", "contents of simulation calculation", and "binding site", since they are not designated as priority items, even conditions that do not satisfy the user presented conditions are displayed.

A price estimation is calculated by defining

25   points in advance for the respective items of the user presented conditions shown in Table 1 and totalizing the points.

The price estimation result is input to the transmission/reception section 2-2. The transmission/reception section 2-2 inputs the received price estimation result to the information management

5   section 2-5. The information management section 2-5 stores the received price estimation result in the storage section 2-6 (S506). The user can refer to the price estimation result by operating the user terminal apparatus 5 and accessing the information management

10   section 2-5.

The user refers to the price estimation result and examines whether the simulation calculation is to be continued or the system is to be ended without executing the simulation calculation. When the simulation

15   calculation should be continued, the user examines whether the simulation calculation should be executed on the basis of the current conditions or re-examines the simulation calculation conditions, and transmits the examination result.

20   The examination result transmitted from the user terminal apparatus 5 is received by the transmission/reception section 2-2 of the user management apparatus 2 (S507).

When the examination result indicates that the

25   simulation calculation should be continued (YES in S508), the user presented conditions are input from the transmission/reception section 2-2 to the estimation

section 2-8 through the calculation control section 2-7.
The estimation section 2-8 estimates the price again on
the basis of the newly input user presented conditions.
The result is transmitted to the matching section 3-1 of

5 the simulation analysis apparatus 3 together with the
user presented conditions (S509).

When the received examination result indicates
that no simulation calculation should be executed, the
system is ended (NO in S508).

10 Table 3 User Presented Conditions Transmitted
to Matching Section

Delivery Time	Price	Contents of Simulation Calculation				Priority Item
		Three-Dimensional Structure	Energy	Property	Docking	
30	400	YES	YES	YES	YES	Delivery time
		YES	YES	YES		
Number of amino acid residues	Number of atoms	Composition	Three-dimensional structure information	Sequence information	Homology	Binding site
100	1500	Amino acid	UNKNOWN	UNKNOWN	UNKNOWN	10
-	60	Organic	UNKNOWN	-	-	
Other condition: Rank is at least A						

For example, when the user refers to the
estimation result and changes the user presented
conditions to those shown in Table 3, the changed

20 conditions are transmitted to the matching section. In
this example, "price" is changed from 200 dollar to 400
dollar, "binding site" is changed from UNKNOWN to KNOWN,
"number of known sites" is set to 10, and "consultant
rank" is designated as at least A.

25   The user presented conditions and price
estimation result transmitted to the matching section
3-1 are transmitted to the transmission/reception

section 4-2 of the consultant management apparatus 4.
Upon receiving the user presented conditions and price
estimation result, the transmission/reception section
4-2 inputs the user presented conditions and automatic

5   price estimation result to the information management
section 4-5. The information management section 4-5
registers the received user presented conditions and
price estimation result in the storage section 4-6.

The consultant accesses the consultant

10   management apparatus 4 and refers to a list of user
presented conditions and automatic price estimation
results.

The consultant selects user presented
conditions and an automatic price estimation result, for

15   which he/she wants to offer consultations, from the list
of user presented conditions and automatic price
estimation results, and inputs and transmits bidding
conditions on the basis of the selected user presented
conditions and automatic price estimation result.

20   The bidding conditions transmitted from the
consultant terminal apparatus 7 are received by the
transmission/reception section 4-2 of the consultant
management apparatus 4 and transmitted to the matching
section 3-1 of the simulation analysis apparatus 3.

25   Table 4   Bidding Conditions from Consultants

Consultant	Delivery Time	Price	Rank	Simulation Method
A	14	500	B	1
B	30	300	A	1
C ·	14	400	A	1

| D | 21 | 300 | B | 2 |
| E | 30 | 200 | C | 1 |

As shown in Table 4, bidding conditions from consultants include, e.g., "consultant", "delivery time", "price", "rank", and "simulation method".

5   Consultants who have referred to the user presented conditions and transmitted bidding conditions are displayed in the "consultant" field.

Delivery times and prices designated by the consultants are displayed in the "delivery time",

10   "price", and "simulation method" fields.

The ranks may be either input by the consultants themselves or automatically displayed by the system.

In the bidding conditions, since the priority

15   item designated in the user presented conditions is "delivery time", bidding conditions that satisfy the delivery time are transmitted to the matching section 3-1.

For example, when the priority item designated

20   in the user presented conditions is "price", bidding conditions that satisfy the designated price are transmitted to the matching section 3-1.

Upon receiving the bidding conditions (S510), the matching section 3-1 compares the user presented

25   conditions with the received bidding conditions, selects bidding conditions that coincide with (match) the user presented conditions (YES in S511), and inquires of the

user terminal apparatus 5 about whether simulation
calculation is to be executed on the basis of the
selected bidding conditions (S512).

In selecting bidding conditions, comparison is
done in the order of priority items (e.g., "delivery
time", "price", "calculation method", and "rank")
designated in the user presented conditions. A
consultant who has presented optimum conditions makes a
successful bid. If no priority item is designated,
comparison is performed in the order of "delivery time",
"price", "calculation method", and "rank". Even if the
conditions do not completely coincide with each other,
optimum conditions for the user presented conditions are
selected. If no bidding conditions coincide with the
user presented conditions, the system is ended (NO in
S511).

Referring to the user presented conditions
shown in Table 3 and the bidding conditions shown in
Table 4, the priority item designated in the user
presented conditions is "delivery time". Hence
comparison is done in the order of "delivery time",
"price", "calculation method", and "rank".

Since the delivery time designated in the user
presented conditions is 30 days, all consultants satisfy
the condition. All consultants except A satisfy the
condition of price. No condition is designated as
"calculation method". When the ranks are compared,

consultants B and C satisfy the condition.

Upon receiving the answer to the inquiry from the user terminal apparatus 5 (S513), the matching section 3-1 determines whether the answer indicates that the user will commission the selected consultant to execute simulation calculation (S514). When the selected consultant is to be commissioned to execute simulation calculation, the simulation conditions are input to the simulation section 3-2 (YES in S515). When the answer indicates that the user will not commission the selected consultant to execute simulation calculation, the system is ended (NO in S515).

Upon receiving the simulation calculation conditions, the simulation section 3-2 first searches for the three-dimensional structure of the target protein (S601).

The simulation section 3-2 has, e.g., a protein three-dimensional structure information DB (not shown), a protein sequence structure DB (not shown), and a homology information DB (not shown). The protein three-dimensional structure information DB stores information of the three-dimensional structures of proteins. The protein sequence structure DB stores information of the sequence structures of proteins. The homology information DB stores information of homology of proteins.

The three-dimensional structure of the target

protein is searched for first by searching the protein three-dimensional structure information DB (S601). If it is determined as a result of search that the target protein is present in the protein three-dimensional

5 structure information DB (YES in S601), protein three-dimensional structure information is acquired (S602).

When the target protein is not present in the protein three-dimensional structure information DB (NO

10 in S601), the sequence information of the target protein is searched for (S603). The sequence information of the target protein is searched for by searching the protein sequence structure DB. If it is determined as a result of search that the sequence information of the target

15 protein is present in the protein sequence structure DB (YES in S603), homology information is searched for. When the sequence information of the target protein is not present in the protein sequence structure DB, the system is ended (NO in S603).

20 Homology information is searched for by searching the homology information DB (S604). If it is determined as a result of search that the sequence information of the target protein is present in the homology information DB (YES in S604), it is determined

25 whether the three-dimensional structure can be estimated by using a method such as homology modeling (S605). If .the sequence information of the target protein is not

present in the homology information DB, the system is ended (NO in S604).

When the three-dimensional structure can be estimated, the estimated protein three-dimensional structure information is acquired (S602). If the three-dimensional structure cannot be estimated, the system is ended. If the calculation is impossible because of the performance of the computer prepared in the simulation section 3-2, the user may be notified of it.

Search of the three-dimensional structure of a molecule as a drug candidate will be described next.

For example, when no three-dimensional structure information is present, it is estimated from sequence information or by using a method of molecular mechanics, molecular dynamics, or molecular orbitals.

For example, the simulation section 3-2 has a ligand molecule three-dimensional structure information DB (not shown) and a molecular formula DB (not shown) of ligand molecules. The ligand molecule three-dimensional structure information DB stores information of the three-dimensional structures of ligand molecules. The molecular formula DB of ligand molecules stores information of the molecular formulas of ligand molecules.

The three-dimensional structure of a molecule as a drug candidate is searched for by searching the

ligand molecule three-dimensional structure information DB (S701). If it is determined as a result of search that the molecule as the drug candidate is present in the ligand molecule three-dimensional structure

5   information DB (YES in S701), the ligand molecule three-dimensional structure information is acquired (S702).

When the molecule as the drug candidate is not present in the ligand molecule three-dimensional

10   structure information DB (NO in S701), the molecular formula of the molecule as the drug candidate is searched for (S703). The molecular formula of the molecule as the drug candidate is searched for by searching the molecular formula DB of ligand molecules.

15   If it is determined as a result of search that the molecular formula of the molecule as the drug candidate is present in the molecular formula DB of ligand molecules, three-dimensional structure initial coordinates are generated (S704). When the molecular

20   formula of the molecule as the drug candidate is not present in the molecular formula DB of ligand molecules (NO in S703), the system is ended.

When the three-dimensional structure initial coordinates are generated, conformations are searched

25   for (S705), and necessary conformations are extracted (S706). The extracted conformations are elaborated (S707). If the three-dimensional structure can be   .

estimated, the estimated three-dimensional structure
information of the molecule as the drug candidate is
acquired (S702). If the calculation is impossible
because of the performance of the computer prepared in
5   the simulation section 3-2, the user may be notified of
it.

Next, using the above-described
three-dimensional structures of the target protein and
the molecule as the three-dimensional structure drug
10   candidate as initial values, simulation calculation is
executed for an item designated as the contents of
simulation calculation in the user presented conditions.

First, the contents of simulation calculation
in the user presented conditions transmitted to the
15   matching section are acquired (S801).

For example, according to the user presented
conditions transmitted to the matching section, which
are shown in Table 3, energy calculation, property
calculation, and docking simulation of each molecule are
20   executed.

Information about binding portions is obtained
by causing the user to input it when the number of
binding portions is known or designated by the user. If
the number of binding sites is unknown, the information
25   is obtained by automatically determining binding
portions equal in number to that designated by the user
at random on a protein.

As the calculation method, the method determined at the time of matching is used.

First, it is determined whether the contents of simulation calculation are designated (S802). If neither energy calculation by the method of molecular orbitals nor docking simulation is designated, the system is ended (NO in S802).

When the contents are designated (YES in S802), it is determined whether the contents of simulation calculation indicate energy calculation by the method of molecular orbitals (S803).

When not energy calculation by the method of molecular orbitals but docking simulation is designated, docking simulation by classical mechanics or QMMM docking simulation, or both of them are directly executed.

When energy calculation by the method of molecular orbitals is designated (YES in S803), energy calculation is executed by using the method of molecular orbitals (S804).

Next, it is determined whether physical quantity calculation is designed as the contents of simulation calculation (S805). When physical quantity calculation is designated (YES in S805), physical quantity calculation is executed (S807). The calculation result is input to the simulation result analysis section 3-3 (S808).

When physical quantity calculation is not
designated (NO in S805), the result of energy
calculation by the method of molecular orbitals is
stored in the simulation result analysis section 3-3

5   (S806).

Next, it is determined whether docking
simulation is designed as the contents of simulation
calculation (S809).

When docking simulation is designated (YES in

10 S809), docking simulation by classical mechanics or QMMM
docking simulation, or both of them are executed (S810
to S815). The result of docking simulation is stored in
the simulation result analysis section 3-3 (S812 and
S815).

15   The simulation result analysis section 3-3
sends a copy of the simulation calculation result to the
consultant who has got the contract for the simulation
calculation through the consultant terminal apparatus 7
(S816).

20   The consultant adds intellectual added value
information such as an analysis result or the
explanation of the result while referring to the
received simulation calculation result and transmits the
intellectual added value information to the simulation

25 result analysis section 3-3.

Upon receiving the intellectual added value
information (S817), the simulation result analysis

section 3-3 temporarily stores it (S818) and transmits the received intellectual added value information and the simulation calculation result to the user terminal apparatus 5 (S819).

5   An example will be described next with reference to Figs. 9 to 12, in which when target protein function control which is effective in the drug design field is to be executed by using the above-described simulation calculation service providing system, pieces

10   of information about portions of the target protein, to which molecules as drug candidates bind, and the difference in affinity to the respective portions are to be collected by a non-member user by way of trial.

The user operates the user terminal apparatus

15   5, activates a browser stored in the storage section, and, for example, designates the address of the user management apparatus 2 on the browser to access the user management apparatus 2 through the network 6.

The authentication/registration section 2-3 of

20   the user management apparatus 2 confirms whether the user who is accessing it has already been registered.

If user registration is not executed yet, a notification representing that the user should be registered is sent, and user registration is performed

25   (S901). The user registration may be charged.

User authentication may be performed after user registration (S902).

When the user is granted permission to use as a result of authentication processing, a window in which simulation conditions and request items related to simulation calculation are to be input is displayed on the display section 5d of the user terminal apparatus 5 that is accessing the user management apparatus 2 (S903). The user inputs desired simulation calculation conditions and request items related to the simulation calculation.

For example, when molecular binding simulation (docking simulation) is to be used, the user inputs simulation conditions and request items related to simulation calculation as shown in Table 1 by using the browser or the like and transmits them to the user management apparatus 2. As described above, user presented conditions include "contents of simulation calculation", "information about molecules to be calculated", "delivery time", "price", and "priority item". The items of the user presented conditions can be added or changed, as needed.

The transmitted simulation conditions and request items are received by the transmission/reception section 2-2 as user presented conditions (S904). The user presented conditions received by the transmission/reception section 2-2 are input to the calculation control section 2-7. The user presented conditions are input from the calculation control

section 2-7 to the estimation section 2-8. The

estimation section 2-8 estimates the price of simulation

calculation on the basis of the received user presented

conditions (S905).

5   Since this calculation is trial calculation,

the calculation scale of simulation calculation to be

executed by the simulation section 3-2 and the time

required for calculation have upper limits. If

calculation in a scale beyond the upper limit is

10   designated, the user is notified of the upper limit

value and that the user presented conditions go beyond

the upper limit (S906).

The estimation result is input to the

transmission/reception section 2-2. The

15   transmission/reception section inputs the received

estimation result to the information management section

2-5. The information management section 2-5 stores the

received price estimation result in the storage section

2-6 (S906). The user can refer to the estimation result

20   by operating the user terminal apparatus 5 and accessing

the information management section 2-5.

The user refers to the estimation result and

examines whether the simulation calculation is to be

continued or the system is to be ended without executing

25   the simulation calculation. When the simulation

calculation should be continued, the user examines

whether the simulation calculation should be executed on

the basis of the current conditions or re-examines the simulation calculation conditions, and transmits the examination result.

This operation may be done by, e.g., displaying the simulation condition input window again and causing the user to input simulation conditions again.

The examination result transmitted from the user terminal apparatus 5 is received by the transmission/reception section 2-2 of the user management apparatus 2 (S908).

When the received examination result indicates that the simulation test calculation should be continued (YES in S908), the simulation trial calculation conditions are input from the transmission/reception section 2-2 to the estimation section 2-8 through the trial calculation section 2-10.

When the received examination result indicates that no simulation test calculation should be executed (NO in S908), the system is ended.

On the basis of the newly input user presented conditions, the estimation section 2-8 executes estimation and determines whether the simulation trial calculation goes beyond the upper limit of the processing capability of the system. If the simulation trial calculation goes beyond the upper limit of the processing capability of the system, and trial

calculation cannot be executed (NO in S909), the system
is ended.

When the simulation trial calculation falls
within the limit of the processing capability of the
5   system, and trial calculation can be executed (YES in
S909), the simulation calculation conditions are input
to the simulation section 3-2 (S910).

Upon receiving the simulation calculation
conditions, the simulation section 3-2 first searches
10   for the three-dimensional structure of the target
protein (S1001).

As described above, the simulation section 3-2
has, e.g., a protein three-dimensional structure
information DB (not shown), a protein sequence structure
15   DB (not shown), and a homology information DB (not
shown). The protein three-dimensional structure
information DB stores information of the
three-dimensional structures of proteins. The protein
sequence structure DB stores information of the sequence
20   structures of proteins. The homology information DB
stores information of homology of proteins.

The three-dimensional structure of the target
protein is searched for by searching the protein
three-dimensional structure information DB (S1001). If
25   it is determined as a result of search that the target
protein is present in the protein three-dimensional
structure information DB (YES in S1001), protein

three-dimensional structure information is acquired (S1002).

When the target protein is not present in the protein three-dimensional structure information DB (NO in S1001), the sequence information of the target protein is searched for (S1003). The sequence information of the target protein is searched for by searching the protein sequence structure DB. If it is determined as a result of search that the sequence information of the target protein is present in the protein sequence structure DB (YES in S1003), homology information is searched for. When the sequence information of the target protein is not present in the protein sequence structure DB (NO in S1003), the system is ended (S1003).

Homology information is searched for by searching the homology information DB (S1004). If it is determined as a result of search that the sequence information of the target protein is present in the homology information DB (YES in S1004), it is determined whether the three-dimensional structure can be estimated by using a method such as homology modeling (S1005). If the sequence information of the target protein is not present in the homology information DB (NO in S1004), the system is ended.

When the three-dimensional structure can be estimated, the estimated protein three-dimensional .

structure information is acquired (S1002). If the
three-dimensional structure cannot be estimated, the
system is ended. If the calculation is impossible
because of the performance of the computer prepared in
5   the simulation section 3-2, the user may be notified of
it.

Search of the three-dimensional structure of a
molecule as a drug candidate will be described next.

For example, when no three-dimensional
10   structure information is present, it is estimated from
sequence information or by using a method of molecular
mechanics, molecular dynamics, or molecular orbitals.

For example, the simulation section 3-2 has a
ligand molecule three-dimensional structure information
15   DB (not shown) and a molecular formula DB (not shown) of
ligand molecules. The ligand molecule three-dimensional
structure information DB stores information of the
three-dimensional structures of ligand molecules. The
molecular formula DB of ligand molecules stores
20   information of the molecular formulas of ligand
molecules.

The three-dimensional structure of a molecule
as a drug candidate is searched for by searching the
ligand molecule three-dimensional structure information
25   DB (S1101). If it is determined as a result of search
that the molecule as the drug candidate is present in
the ligand molecule three-dimensional structure

information DB (YES in S1101), the ligand molecule three-dimensional structure information is acquired (S1102).

When the molecule as the drug candidate is not present in the ligand molecule three-dimensional structure information DB (NO in S1101), the molecular formula of the molecule as the drug candidate is searched for (S1103). The molecular formula of the molecule as the drug candidate is searched for by searching the molecular formula DB of ligand molecules.

If it is determined as a result of search that the molecular formula of the molecule as the drug candidate is present in the molecular formula DB of ligand molecules (YES in S1103), three-dimensional structure initial coordinates are generated (S1104). When the molecular formula of the molecule as the drug candidate is not present in the molecular formula DB of ligand molecules (NO in S1103), the system is ended.

When the three-dimensional structure initial coordinates are generated (S1104), conformations are searched for by using the method of molecular mechanics or molecular dynamics (S1105), and necessary conformations are extracted (S1106). The extracted conformations are elaborated by the method of molecular orbitals (S1107). If the three-dimensional structure can be estimated, the estimated three-dimensional structure information of the molecule as the drug

- 56 -

candidate is acquired (S1102). If the calculation is impossible because of the performance of the computer prepared in the simulation section 3-2, the user may be notified of it.

5 　　　　　Next, using the above-described three-dimensional structures of the target protein and the molecule as the three-dimensional structure drug candidate as initial values, simulation calculation is executed for an item designated as the contents of

10 simulation calculation in the user presented conditions.

　　　　　First, the contents of simulation calculation in the user presented conditions transmitted to the matching section are acquired (S1201).

　　　　　For example, according to the user presented

15 conditions transmitted to the matching section, which are shown in Table 3, energy calculation, property calculation, and docking simulation of each molecule are executed.

　　　　　Information about binding portions is obtained

20 by causing the user to input it when the number of binding portions is known or designated by the user. If the number of binding sites is unknown, the information is obtained by automatically determining binding portions equal in number to that designated by the user

25 at random on a protein.

　　　　　As the calculation method, the method determined at the time of matching is used.

First, it is determined whether the contents of simulation calculation are designated (S1202).

If neither energy calculation by the method of molecular orbitals nor docking simulation is designated, the system is ended (S1202).

When the contents are designated (YES in S1202), it is determined whether the contents of simulation calculation indicate energy calculation by the method of molecular orbitals (S1203).

When not energy calculation by the method of molecular orbitals but docking simulation is designated, docking simulation by classical mechanics or QMMM docking simulation, or both of them are directly executed.

When energy calculation by the method of molecular orbitals is designated (YES in S1203), energy calculation is executed by using the method of molecular orbitals (S1204).

Next, it is determined whether physical quantity calculation is designed as the contents of simulation calculation (S1205). When physical quantity calculation is designated (YES in S1205), physical quantity calculation is executed (S1207). The calculation result is input to the simulation result analysis section 3-3 (S1208).

When physical quantity calculation is not designated (NO in S1205), the result of energy .

- 58 -

calculation by the method of molecular orbitals is
stored in the simulation result analysis section 3-3
(S1206).

Next, it is determined whether docking
5   simulation is designed as the contents of simulation
calculation (S1209).

When docking simulation is designated (YES in
S1209), docking simulation by classical mechanics or
QMMM docking simulation, or both of them are executed
10   (S1210 to S1215). The result of docking simulation is
stored in the simulation result analysis section 3-3
(S1212 and S1215).

The simulation result analysis section 3-3
sends a copy of the simulation calculation result to the
15   consultant who has got the contract for the simulation
calculation through the consultant terminal apparatus 7
(S1216).

The consultant adds intellectual added value
information such as an analysis result or the
20   explanation of the result while referring to the
received simulation calculation result and transmits the
intellectual added value information to the simulation
result analysis section 3-3.

Upon receiving the intellectual added value
25   information (S1217), the simulation result analysis
section 3-3 temporarily stores it (S1218) and transmits
the received intellectual added value information and .

the simulation calculation result to the user terminal apparatus 5 (S1219).

According to the present invention, the user need not purchase any computer or software by himself/herself. The user need not prepare any server to be connected to the Internet, either, and can use simulation through the network. For this reason, the convenience of use of simulation can be increased for temporary users and non-experts. Additionally, since change/upgrading of application software can be done by only the Internet provider, a user-friendly system can be implemented.

The user who uses this simulation calculation service system can select a consultant who can solve problems. When the user requests simulation, he/she designates a consultant having a necessary technical capability. The simulation calculation service system selects a consultant on the basis of the priority item designated by the user.

The user inputs a problem to be subjected to simulation calculation by using the user terminal apparatus. The provider manages the server system. The consultant refers to user presented conditions by using the consultant terminal apparatus, inputs bidding conditions within a predetermined period, executes simulation calculation by using the server system managed by the operator, and examines the analysis

result.

The user can easily input a simulation request
by using input means such as a browser and graphical
user interface.

5   The user can change simulation calculation
conditions in consideration of an estimation result.
The user can also use the system by way of trial.

Since the system provider can flexibly cope
with the maintenance of the system and any accident, the
10   robustness of the system increases. Computer makers and
Internet providers can prompt to find new users.

Furthermore, requirements between the user and
the consultant can match. Problems of research workers
can be solved by using a simulation technology
15   established by simulation experts or IT providers and a
developed simulation system. For these reasons, a new
simulation technology can easily be introduced. In
addition, business opportunities using simulation and
market creation opportunities can be increased.

20   Since opportunities to use the simulation
system by way of trial are given to non-member users,
the opportunities to acquire users can be increased.

The system provider can efficiently operate
resources such as computer hardware and software. The
25   system provider can also efficiently collect investments
for computer hardware and software.

The consultant can receive the consultant fee.

The Internet provider can obtain new Internet users.

The consultant can present questions, individual proposals, and individual estimations within a predetermined period on the basis of user presented

5   conditions.   On the other hand, the user can respond to them by sending answers to the questions or sending questions to the individual proposals or individual estimations.   The user can change user presented conditions on the basis of the result of response.   By

10   the above-described response, the user can know the price of simulation calculation in advance and determine by referring to the price whether simulation should be executed.